

# Morphology of critically sized crystalline nuclei at shear-induced crystal nucleation in amorphous solid

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## Abstract

© 2017 The Society of Rheology. In this work, we study morphological characteristics of the critically sized crystalline nuclei at initial stage of the shear-induced crystallization of a model single-component amorphous (glassy) system. These characteristics are estimated quantitatively through statistical treatment of the nonequilibrium molecular dynamics simulation results for the system under steady shear at various (fixed) values of the shear rate  $\dot{\gamma}$  and at different temperatures. It is found that the sheared glassy system is crystallized through nucleation mechanism. From the analysis of time-dependent trajectories of the largest crystalline nuclei, the critical size  $n_c$  and the nucleation time  $\tau_c$  were defined. It is shown that the critically sized nuclei in the system are oriented within the shear-gradient  $xy$ -plane at moderate and high shear rates; and a tilt angle of the oriented nuclei depends on the shear rate. At extremely high shear rates and at shear deformation of the system more than 60%, the tilt angle of the nuclei tends to take the value  $\approx 45^\circ$  respective to the shear direction. We found that this feature depends weakly on the temperature. Asphericity of the nucleus shape increases with increasing shear rate that is verified by increasing value of the asphericity parameter and by the contour of the pair distribution function calculated for the particles of the critically sized nuclei. The critical size increases with increasing shear rate according to the power-law,  $n_c \propto (\dot{\gamma} \tau_c)^{1/3}$ , whereas the shape of the critically sized nucleus changes from spherical to the elongated ellipsoidal. We found that the  $n_c$ -dependencies of the nuclei deformation parameter evaluated for the system at different temperatures and shear rates are collapsed into unified master-curve.

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